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THE DEVELOPMENT AND APPLICATION OF SCDAP-3D©

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ABSTRACT

The SCDAP-3D© computer code (Coryell 2001) has been developed at the Idaho National Engineering & Environmental Laboratory (INEEL) for the analysis of severe reactor accidents. A prominent feature of SCDAP-3D© relative to other versions of the code is its linkage to the state-of-the-art thermal/hydraulic analysis capabilities of RELAP5-3D©. Enhancements to the severe accident models include the ability to simulate high burnup and alternative fuel, as well as modifications to support advanced reactor analyses, such as those described by the Department of Energy's Generation IV (GenIV) initiative. Initial development of SCDAP-3D© is complete and two widely varying but successful applications of the code are summarized. The first application is to large break loss of coolant accident analysis performed for a reactor with alternative fuel, and the second is a calculation of International Standard Problem 45 (ISP-45) or the QUENCH 6 experiment.

INTRODUCTION

The SCDAP-3D© code evolved from the RELAP5 and SCDAP/RELAP5 codes developed at the Idaho National Engineering & Environmental Laboratory (INEEL) under the primary sponsorship of the U.S. Nuclear Regulatory Commission (NRC). Development of the RELAP5 code series began at the INEEL in 1975, while SCDAP development was initiated in the early 1970's with an active linkage to RELAP5 in 1979. Following the accident at Chernobyl, the U.S. Department of Energy (DOE) began a re-assessment of the safety of its test and production reactors, and chose RELAP5 and SCDAP/RELAP5 as the analytical tools for system safety analysis because of their wide spread acceptance and ease of application to such widely varying systems. Systematic safety analyses were performed for the N reactor at Hanford, the K and L reactors at Savannah River, the Advanced Test Reactor (ATR) at INEEL, the High Flux Isotope Reactor (HFIR) and Advanced Neutron Source (ANS) at Oak Ridge, and the High Flux Beam Reactor at Brookhaven. DOE also chose RELAP5 for the independent safety analysis of the New Production Reactor (NPR) before that program was cancelled.

The application of SCDAP/RELAP5 and RELAP5 to these widely varying reactor designs demanded new modeling capabilities, including non-light water reactor (LWR) materials and geometry. These widely varying demands were met by maintaining a single source with options that could be selected or deselected at compilation. In this fashion both NRC and DOE users could receive maximum benefit from the others development efforts. After the transmittal of SCDAP/RELAP5 Mod3.3 to the NRC, it became clear, however, that the efficiencies realized by the maintenance of a single source code for use by both NRC and DOE were being overcome by the extra effort required to accommodate sometimes conflicting goals and requirements. The codes were therefore "split" into two versions, SCDAP/RELAP5 Mod3.3 for the NRC and SCDAP-3D© for DOE. The SCDAP-3D© code maintained all of the capabilities and validation history of the predecessor codes, plus the added capabilities sponsored by the DOE.

SCDAP-3D© is capable of modeling a wide range of system configurations from single pipes to experimental facilities to full-scale reactor systems. The configurations can be modeled using an arbitrary number of fluid control volumes and connecting junctions, heat structures, core components, and system components. Flow areas, volumes, and flow resistances can vary with time through either user-control or models that describe the changes in geometry (like those associated with damage in the core). System structures can be modeled with heat structures, core components, or debris models. Other system components available to the user include pumps, valves, electric heaters, jet pumps, turbines, separators, and accumulators. Models to describe selected processes, such as reactor kinetics, control system response, and tracking noncondensable gases, can be invoked through user control.

DEVELOPMENT

A prominent attribute that distinguishes SCDAP-3D© from SCDAP/RELAP5 is associated with its linkage to the thermal/hydraulic analysis capabilities of RELAP5-3D©. These features include a fully integrated, multi-dimensional thermal-hydraulic and kinetic modeling capability that removes any restrictions on the applicability of the code to the full range of postulated reactor accidents. Other enhancements include a new matrix solver, new water properties, and improved time advancement for greater robustness.

Enhancements to the severe accident models include the ability to simulate high burnup and alternative fuel, as well as modifications to support advanced reactor analyses, such as those described by DOE's GenIV initiative. Modifications have been performed to better model analyses of experimental facilities, such as the FZK QUENCH facility, as well as steam generator tube rupture analyses. An interface to the RELAP5-3D© graphical user interface (GUI) has also been added. Together with the modeling capabilities of RELAP5-3D©, these enhancements make the SCDAP-3D© code the most powerful analytical tool of its kind available.

APPLICATION OF SCDAP-3D© TO THO_2-UO_2 LARGE BREAK LOCA ANALYSIS

Thoria-urania (ThO_2-UO_2) fuel can be operated to a relatively high burnup level, and may have the potential to improve fuel cycle economics (allow higher sustainable plant capacity factors), improve fuel performance, increase proliferation resistance, and be a more stable and insoluble waste product than traditional UO_2 fuel (MacDonald and Herring 2000). To better understand the impact of this advanced fuel on reactor safety, a large break LOCA analysis has been performed to compare the response of thoria-urania fuel with traditional UO2 fuel.

Although SCDAP-3D© has been successfully applied to large break LOCA analyses for many years, it has been necessary to extend the code to use a mixed thoria-urania fuel in analyses of this type. Extensions were made to allow the code user to describe both high burnup fuel and ThO_2-UO_2 fuel, and material property correlations were added to calculate ThO_2-UO_2 fuel thermal conductivity, heat capacity, density, and emissivity. Other extensions include the ability to model the effect that hydrogen dissolved in the Zircaloy cladding has on the behavior of the cladding, and the ability to define the axial distribution in the radial power profile. This addition gives the code the ability to model the large axial variation in radial power peaking factors for fuel rods with high burnup. For example, in a fuel rod with a burnup of 33,000 MWd/MTU the radial peaking factor may vary from 2.0 at the bottom of the fuel rod to 3.0 at the mid-elevation of the fuel rod.

The Seabrook pressurized water reactor (PWR) was selected as the framework for comparing the performance of ThO_2-UO_2 and 100% UO_2 fuels during a large break LOCA. This PWR was analyzed in an NRC sponsored study to evaluate the possibility of relaxing the time to isolate the containment in the event of a large break LOCA (Jones et al. 1992). The Seabrook PWR has four loops in its primary coolant system. During normal power production, the reactor produces 3389 MW of thermal power. The pressure in the primary coolant system during normal operation is 15.17 MPa (2200 psi). Each coolant loop has a steam generator and a pump. One of the four loops also has a pressurizer. The safety systems on the reactor include an accumulator on each cold leg with the capability to inject 24 m^3 (850 ft^3) of water by nitrogen back pressure when the primary coolant system pressure decreases to value less than 4.14 MPa. The Seabrook PWR has a core composed of 193 17x17-type fuel assemblies. Except for the composition of the fuel, the characteristics of the fuel assemblies for the ThO_2-UO_2 and 100% UO_2 fuels were identical. The characteristics of the fuel assemblies are described in Table 1. The ThO_2-UO_2 fuel was composed of 70% ThO_2 and 30% UO_2.

Table 1. Characteristics of the fuel assemblies in the Seabrook PWR.

Characteristic	Value
Outer diameter of fuel pellets (mm)	8.19
Outer diameter of fuel rod cladding (mm)	9.50
Thickness of cladding (mm)	0.57
Composition of fuel	100%UO_2 or 70%ThO_2-30% UO_2
Plenum length (m)	0.165
Height of stack of fuel pellets (m)	3.66
Density of fuel (fraction of theoretical maximum)	0.951
Composition of fill gas	100% He
Pressure of fill gas (MPa)	2.52

The power in the fuel rods was defined according to the Technical Specifications for the Seabrook PWR (Jones et al. 1992). According to these specifications, the average linear heat generation in the reactor core is defined to be 17.83 kW/m and the maximum linear heat generation rate in the reactor core is defined to be a factor of 2.32 greater than the average linear heat generation rate. In addition, the core thermal power is defined to be 102% of its rated thermal power. Thus, the peak linear heat generation rate in the reactor core is 1.02x2.32x17.83 kW/m, which equals 42.19 kW/m. According to the Technical Specifications, the axially averaged linear heat generation in the hottest rod is defined to be a factor of 1.49 greater than the axially averaged average linear heat generation rate in the core. The axial power is defined to have a chopped, symmetric cosine distribution. The ratio of the peak to average linear heat generation in the hottest rod is equal to 1.557, and this ratio for the other rods in the reactor core is defined to be 1.47. The radial power distribution in the reactor core was as follows. The linear power in center four fuel assemblies was a factor of 1.49 greater than the core average linear power. The linear power in the 77 fuel assemblies outward from the center four fuel assemblies was 4.9% greater than the core average linear power. The linear power in the outer 112 fuel assemblies was 94.9% of the core average linear power.

The behavior of the ThO_2-UO_2 and 100% UO_2 fuels at the position of the hottest rod in the reactor core are compared as a function of burnup in Table 2. Although it is highly unlikely that a fuel rod would stay in the position of the hottest fuel rod until an axially averaged burnup of 30,470 MWd/MTU, nevertheless this condition was assumed in order to calculate the earliest possible rupture of fuel rod cladding during a large break LOCA.

Table 2. Comparison of behavior of ThO_2-UO_2 and 100% UO_2 fuel for hottest fuel rod in reactor core

Axially averaged burnup	**Centerline temperature at elevation of peak power (K)**		**Fission gas release (%)**		**Fuel rod internal pressure (MPa)**	
(MWd/MTU)	100%UO_2	ThO_2-UO_2	100%UO_2	ThO_2-UO_2	100%UO_2	ThO_2-UO_2
870	1904	1921	0.60	0.63	9.02	8.68
10,370	1773	1748	2.14	2.00	9.37	9.00
20,420	1890	1862	10.40	9.49	13.27	12.44
30,470	1996	1958	22.98	20.96	21.73	19.38

The entire primary coolant system of the Seabrook PWR was modeled by SCDAP-3D©. Three parallel stacks of nine control volumes represented the fluid in the reactor core region, with cross-flow between the stacks taken into account. The first stack of control volumes represented the fluid in the center four fuel assemblies, the second represented the fluid in the 77 fuel assemblies outward from the center four fuel assemblies, and the third represented the fluid in the outer 112 fuel assemblies of the reactor core. The broken loop in the primary coolant system was represented by one network of control volumes and the three unbroken loops were represented by another network of control volumes. The steam generator was represented by eight control volumes, the hot leg by four control volumes, and the cold leg by ten control volumes. Each loop had control volumes to represent a reactor coolant system pump and an accumulator. The broken loop also included a representation of the pressurizer. The reactor vessel downcomer was represented by two parallel stacks of seven control volumes, with cross-flow taken into account. The reactor containment was represented by one control volume.

The large break LOCA was assumed to be a complete, double-ended, offset-shear break in the piping of the cold leg of the coolant system loop with the pressurizer. The Emergency Core Coolant System (ECCS) was assumed to not operate and the primary system coolant pumps are assumed to continue to operate after the initiation of the break.

The transient reactor fission power was calculated using the SCDAP-3D© reactor kinetics model and the transient decay heat was calculated using models appropriate for each composition of fuel. In order to calculate the transient reactor fission power, a table defining reactivity as a function of moderator density was input to the reactor kinetics model. The relation of reactivity to moderator density was assumed to be the same for both compositions of fuel. For the case of 100% UO_2 fuel, the transient decay heat was calculated by the SCDAP-3D© decay heat model. For the case of 70%ThO_2-30%UO_2 fuel, the transient decay heat was obtained from a reactor physics calculation (Herring 2000) and input to the code as a table of power versus time. At 30 s and 60 s after the initiation of the accident, the ratios of decay heat in the 70%ThO_2-30%UO_2 fuel to that in 100% UO_2 fuel were 1.043 and 1.048, respectively.

The performance of the 70%ThO_2-30%UO_2 and 100%UO_2 fuel rods during the large break LOCA were similar. The transient coolant pressure at the center of the reactor core is shown in Figure 1 for the case of 70%ThO_2-30%UO_2 fuel. The transient pressure for the case of UO_2 fuel was similar.

The maximum cladding temperatures in the reactor core for the two fuel compositions are compared in Figure 2. For both fuel compositions, the maximum cladding temperatures occurred in the fuel rods with the highest linear fuel rod power and an axially averaged burnup of 30,470 MWd/MTU. In the period from the start of the accident to 34 s after the start of the accident, the cladding temperatures for the two fuel compositions were almost identical. After 34 s, maximum cladding temperature for the 100%UO_2 case was somewhat greater than that for the 70%ThO_2-30%UO_2 case. For both fuel compositions, the heatup of the reactor core was mitigated by the injection of water from the accumulators beginning at 13 s. This injection of water limited the maximum cladding temperature for both cases to a value less than the limit of 1476 K (2200°F) established by the USNRC in 10CFR Part 50.46 (Shotkin et al. 1987). For both fuel compositions, the combination of cladding heatup and depressurization of the primary coolant system was calculated to cause the cladding of some of the fuel rods in the reactor core to balloon and rupture. The time for first rupture of the fuel rod cladding was calculated to be 33 s for both fuel compositions. For both cases, cladding ballooning and rupture was calculated to occur only in the four fuel assemblies in the center of the reactor core.

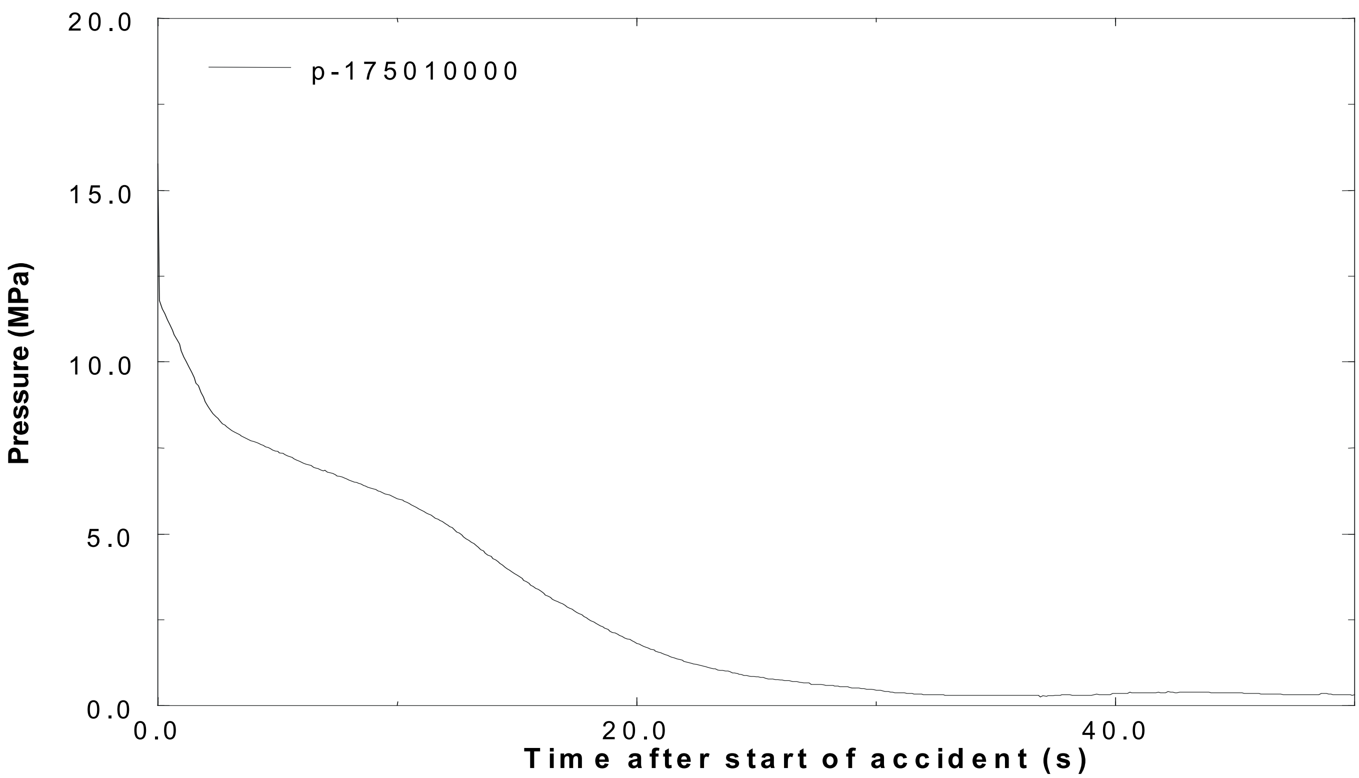

Figure 1. Transient coolant pressure at center of reactor core for case of 70% ThO2 - 30% UO2

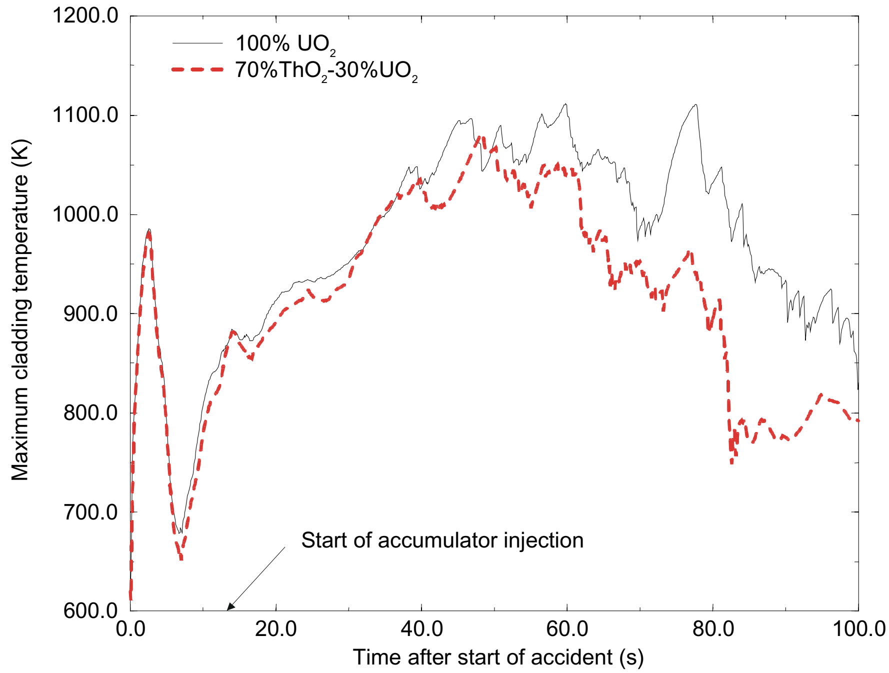

Figure 2. Maximum fuel rod cladding temperature during large break LOCA.

APPLICATION OF SCDAP-3D© TO QUENCH FACILITY

One of the most significant and dramatic accident management actions that can be taken to terminate a Light Water Reactor (LWR) severe accident is to inject ECC water to cool the uncovered and potentially degraded core. However, analysis of the TMI-2 accident, as well as both in-pile and out-of-pile experiments have shown that the injection of water can initially cause significant additional damage to the uncovered core, and that there will actually be an enhanced oxidation of the Zircaloy cladding with a resulting increase in core temperature, hydrogen production, and fission product release.

In an effort to better understand these phenomena the Forschungszentrum Karlsruhe (FZK) has started the QUENCH program. This program has the objectives of:

- Providing an experimental data base to assist in the development of mechanistic models,
- Examining the behavior of reactor core elements under different flooding conditions, and
- Improving the understanding of water injection at different stages of core degradation.

The QUENCH-06 experiment, performed on December 13, 2000, was designated as an OECD/NEA International Standard Problem (ISP-45) to provide a broad comparison between experimental and analytical results derived from various computer codes (Hering, 2001a). ISP-45 was a "blind" standard problem, meaning that only the inlet and boundary conditions were provided to the participants, until after the calculated results were provided to FZK. While a blind ISP is useful in comparing analytical results from various codes, it is less useful in understanding the behavior and interactions of various models within a given code. Although SCDAP-3D© was successfully used to participate in the blind calculation, the results reported here are from a subsequent analysis performed to assess the severe accident and reflood models.

The QUENCH facility design is intended to allow the operators to heat the fuel rod simulators in a oxidizing environment while controlling steam and argon flow, and when the desired amount of oxidation has occurred, to initiate a reflood at any desired reflood rate, while measuring parameters such as hydrogen production, temperatures, and flow rates. The QUENCH test bundle, shown in Figure 3, consists of a test section with electrically heated fuel rod simulators, and supply systems for water, steam, and argon. Superheated steam mixed with argon enters the test bundle at the bottom end. The steam, argon, and hydrogen off-gas produced by the oxidation process exits the bundle from the upper end of the bundle. This effluent is then taken by a water-cooled pipe to the measurement section, where steam is separated from noncondensable gases, so that each can be measured. During the quench phase of the experiment, the reflood water is injected into the bottom of the test bundle. In addition, argon is injected into the top of the bundle to sweep hydrogen to the measurement systems.

The QUENCH-06 experiment was intended to examine the response of a pre-oxidized bundle to flooding occurring at the onset of the temperature excursion due to oxidation. The water injection rate was approximately 1.5 cm/s at the bottom of the bundle and the maximum ZrO2 thickness at the initiation of reflood was approximately 250 µm. Previous experiments in this facility have found that this amount of oxide will experience cracking and spalling under reflood conditions.

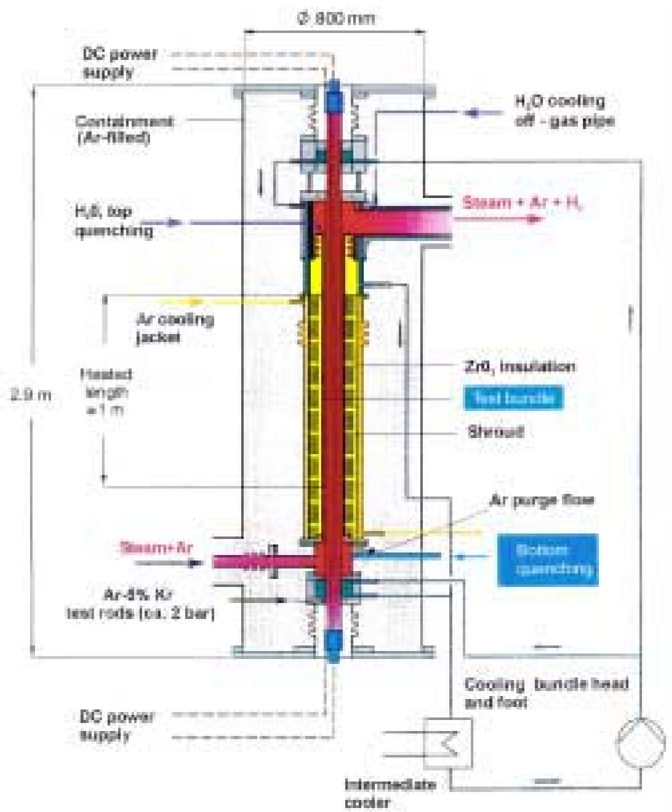

Figure 3 QUENCH test section (courtesy FZK)

The test section consists of 21 fuel rod simulators in a square array, with the corner position occupied by instrumentation rods and the center position occupied by an unheated simulator rod, as shown in Figure 4. The QUENCH bundle is enclosed by a Zircaloy liner, and insulated by a ZrO_2 shroud. The outer boundary of the ZrO_2 shroud is cooled by a jacket, with a counter-current flow of argon providing the heat sink. As was seen in Figure 3, the ZrO_2 insulation extends over the inlet section and the heated length, but is missing above the heated length of the simulators. This section of the test section, not insulated by ZrO_2, will be shown to be significant to the thermal response of the simulator.

All of the fuel rod simulators have cladding typical of Pressurized Water Reactor (PWR) cladding in both material and dimensions. The heated simulators have a heated length of approximately one meter with sections of molybdenum and copper electrode at each end as shown in Figure 5. Surrounding the electrodes are alumina (Al_2O_3) annular rings (solid in the unheated simulator) extending radially to the typical fuel pellet dimensions, and simulating the effects of the fuel pellets. The gas gap is filled with helium at slightly above system pressure, and is connected to a gas reservoir outside the test section, to prevent cladding deformation.

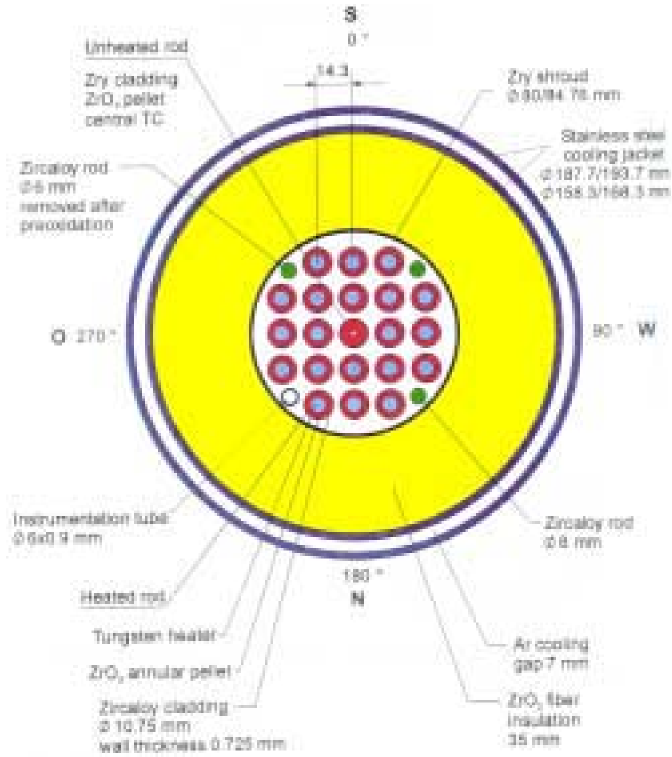

Figure 4. QUENCH test bundle (Courtesy FZK)

Two code modifications to SCDAP-3D© were necessary in order to model conditions which are unique to the QUENCH facility. These code changes include modifications to model the lack of ZrO2 shroud above the heated length and a new approach to distributing power over the length of the QUENCH fuel rod simulators.

The first modification was required because of the necessity of modeling the entire length of the fuel rod simulator, from inlet to outlet, rather than the more typical approach of modeling just the heated length. Although most components in a PWR core, extend over the entire height of the core, the ZrO2 shroud around the QUENCH test bundle extends only to the top of the heated length. The SCDAP-3D© code was modified such that input can be used to specify the extent of the upper electrode, and the thermal conductivity of the ZrO2 shroud was set to a very high number over the extent of the upper electrode.

The measurement of power delivered to the QUENCH simulators is the drop in voltage across the entire test bundle. For this reason FZK (Hering, 2001b) recommended the implementation of a new power distribution model that would distribute the power, not along a fixed axial power profile, but over the entire length of the simulator, molybdenum and copper electrodes, by a temperature dependent function. This method calculates the resistance as a function of temperature over the entire length of the simulator, adds an input resistance for power losses over the contacts and wiring outside the test bundle, and distributes the power over the modeled length. While this approach allows the power to be distributed axially in a more physical and accurate manner, it applies additional emphasis on the necessity of accurately calculating the thermal profile. Indeed, since the resistance of the electrodes increases with increasing temperature, an over-prediction of temperature at any location leads to an increased power at that location, which then obviously provides a positive feedback effect.

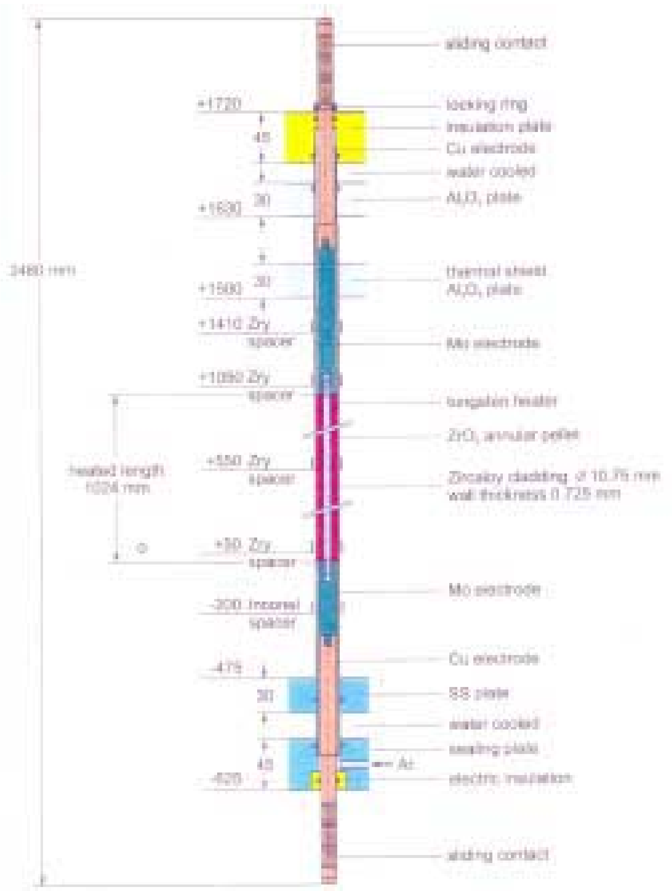

Figure 5 QUENCH fuel rod simulator (courtesy FZK)

The nodalization used to simulate the QUENCH facility is shown in Figure 6. As shown in this figure, there were 3 separate time-dependent volumes, each of which were used to specify the boundary conditions of steam, argon, and quench water. These volumes were then connected to the inlet plenum by time-dependent junctions, allowing the user to specify the flow rates from each volume. This inlet plenum allows mixing prior to the inlet to the test bundle, which is modeled by a stack of 17 vertical volumes, which allows the code to model the upper and lower electrodes, as well as the heated length of the simulators. Not shown is a stack of volumes providing a boundary condition for the cooling jacket of the test bundle, which consists of a counter-current flow of argon at constant temperature.

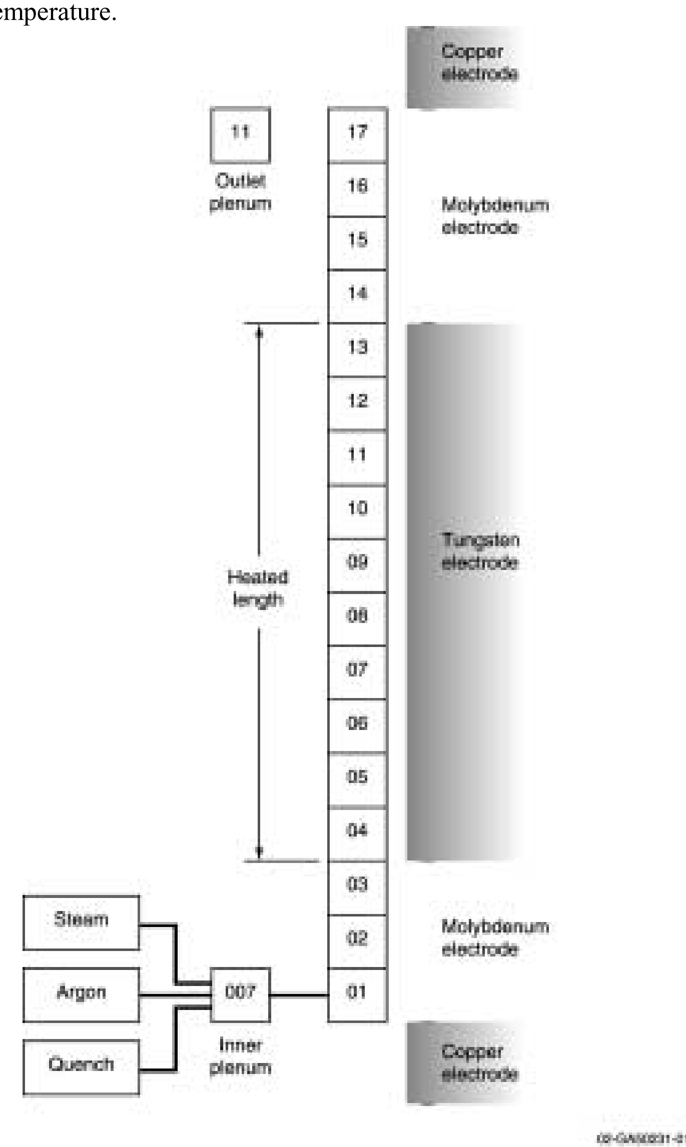

Figure 6 Nodalization of QUENCH facility

Figures 7 and 8 compare the cladding surface temperature calculated at an elevation 650 and 850 mm above the bottom of the heated length, respectively, with thermocouple measurements at the same elevation. These responses are typical of that experienced over the entire heated length, in that the initial heatup rate was modeled as being too slow, but that by 3400 s the calculation overtakes the measured response and follows very nicely until reflood initiation. It is assumed that the discrepancy during the initial oxidation period is a result of an inaccurate specification of the initial conditions. At time zero, the experiment had, obviously, already initiated a transient, with a consequent increased energy in the fuel rod simulator internals, while the calculation was initiated at steady state conditions (due to lack of information of conditions prior to time zero).

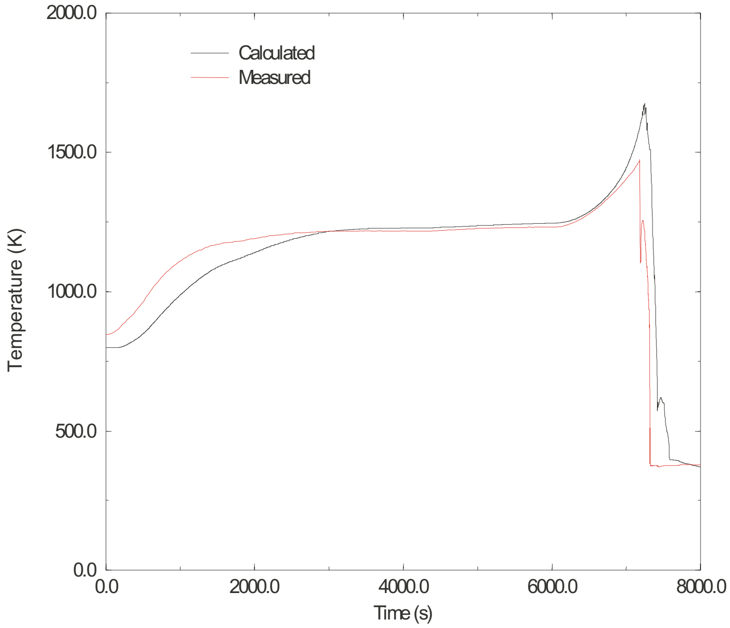

Figure 7 Cladding surface temperatures at 650 mm

These figures also illustrate the tendency of SCDAP-3D© to predict heat generation due to oxidation during the temperature excursion that occurs during reflood. It has been hypothesized that this slight over prediction is a result of the code assuming that the entire metal surface at an axial node is exposed, rather than just cracking the oxide with a consequent exposure of slightly less fresh Zircaloy surface. However a more physical model will require additional information from facilities such as QUENCH, and the implementation of that information into computer models.

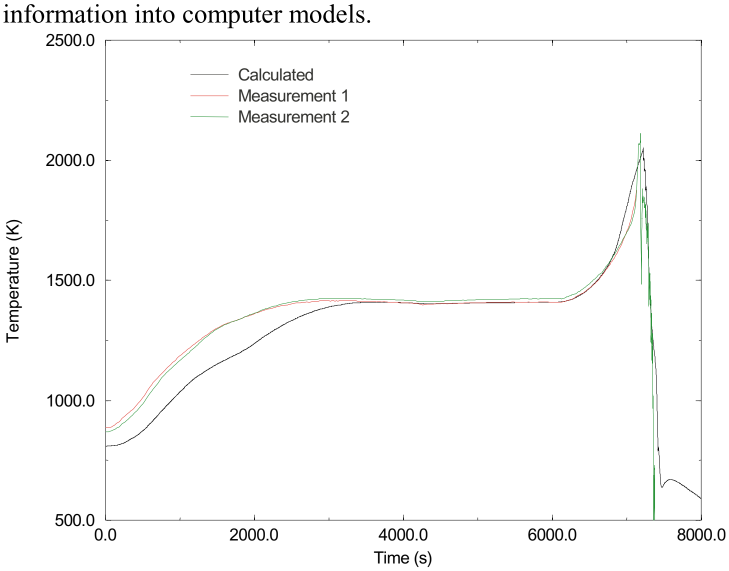

Figure 8 Cladding surface temperatures at 850 mm

Figure 9 shows the cumulative hydrogen production calculated for the QUENCH-06 transient. As could be expected from the close match of temperatures, the hydrogen production matches very well prior to reflood initiation at 7170 s. However, after reflood initiation, SCDAP-3D© predicts significant additional hydrogen production (~50 g), while the initial survey of the experiment reported that only an additional 4.8 g if hydrogen were produced during the reflood. Based upon the significant temperature excursions measured during reflood, the measured hydrogen would appear to be suspect.

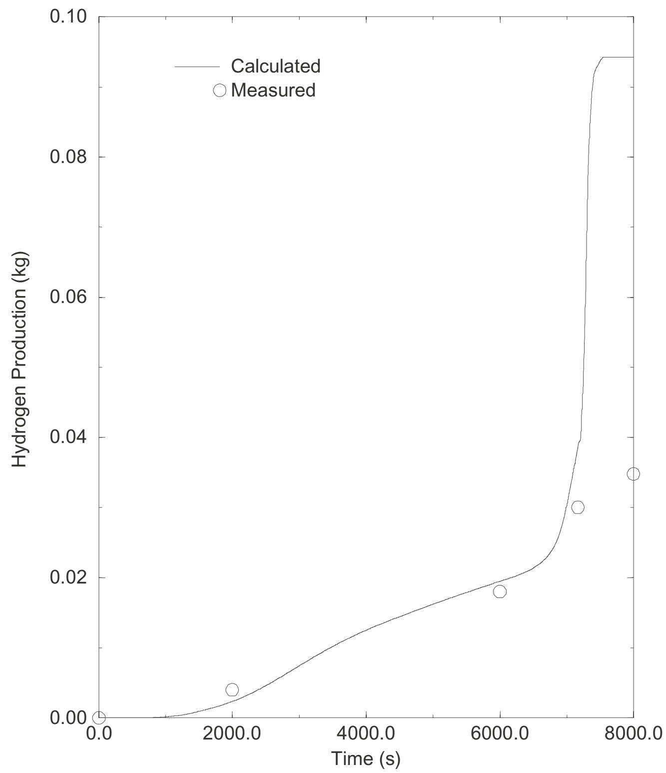

Figure 9 QUENCH-06 cumulative hydrogen production

CONCLUSIONS

The SCDAP-3D© computer code has been generated as the result of the merger of severe accident analysis capability developed in response to U.S. NRC and DOE reactor analysis needs, with the thermal-hydraulic code RELAP-3D© to provide a significantly enhanced reactor safety analysis tool. This code has been applied to a wide variety of analyses, of which two have been described in this paper. These applications, the analysis of a large break loss of coolant accident with alternative fuels, and the analysis of an experimental facility examining accident management issues, illustrate to a small degree, the capability provided by this merger.

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The authors gratefully acknowledge the assistance of Eduardo Honaiser (University of Florida) in the initial development of the QUENCH input model. We would also like to acknowledge the invaluable assistance of the staff at Forschungszentrum Karlsruhe (FZK), particularly Wolfgang Hering and Christoph Homann, in describing the QUENCH facility, and in discussing modifications needed for SCDAP-3D©.

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